

UMPK of E. coli

Contacts of ligands UDP in PDB entry 2BND

The Structure Of E.Coli Ump Kinase In Complex With Udp; P.Briozzo, C.Evrin,
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Lig.1 Residues in contact with ligand UDP1242A in PDB entry 2BND

Legend:

Dist - nearest distance (Å) between atoms of the ligand and the residue

Surf - contact surface area (Å²) between the ligand and the residue

HB - hydrophilic-hydrophilic contact (hydrogen bond)

Arom - aromatic-aromatic contact

Phob - hydrophobic-hydrophobic contact

DC - hydrophobic-hydrophilic contact (destabilizing contact)

+/- - indicates presence/absence of a specific contacts

* - indicates residues contacting ligand by their side chain
(including CA atoms)

Residue		Dist	Surf	Specific contacts			
				HB	Arom	Phob	DC
15A	LYS*	2.6	33.1	+	-	-	-
17A	SER*	2.8	13.5	+	-	-	-
18A	GLY	2.7	26.9	+	-	-	-
19A	GLU*	3.3	4.7	+	-	-	-
56A	GLY*	3.5	1.2	-	-	-	-
57A	GLY*	3.0	18.1	+	-	-	-
58A	GLY	2.9	17.0	+	-	-	-
61A	PHE	4.0	4.5	-	-	-	+
62A	ARG*	2.7	58.4	+	-	-	+
63A	GLY*	2.8	16.3	+	-	-	-
64A	ALA	5.2	0.3	+	-	-	-
73A	ARG*	4.6	2.4	+	-	-	-
76A	GLY	4.4	0.5	+	-	-	-
77A	ASP*	2.6	62.1	+	-	-	+
80A	GLY*	3.0	25.1	-	-	-	+
81A	MET*	3.5	16.4	-	-	+	+
84A	THR*	3.7	22.7	-	-	+	-
137A	GLY*	3.9	12.1	-	-	-	-
138A	THR*	2.6	41.4	+	-	-	+
140A	ASN	2.7	25.8	+	-	-	+
141A	PRO*	3.5	1.7	-	-	-	+
142A	PHE	3.8	0.2	+	-	-	-
143A	PHE*	2.9	40.9	+	-	-	+
144A	THR*	3.5	27.0	-	-	-	+
145A	THR*	2.8	55.7	+	-	+	-

Lig.2 Residues in contact with ligand UDP1242B in PDB entry 2BND

Legend:

Dist - nearest distance (Å) between atoms of the ligand and the residue

Surf - contact surface area (Å²) between the ligand and the residue

HB - hydrophilic-hydrophilic contact (hydrogen bond)

Arom - aromatic-aromatic contact

Phob - hydrophobic-hydrophobic contact

DC - hydrophobic-hydrophilic contact (destabilizing contact)

+/- - indicates presence/absence of a specific contacts

* - indicates residues contacting ligand by their side chain
(including CA atoms)

Residue	Dist	Surf	Specific contacts				DC
			HB	Arom	Phob	DC	
15B LYS*	3.1	34.1	+	-	-	-	
17B SER*	3.5	12.6	+	-	-	-	
18B GLY	3.1	14.7	+	-	-	-	
19B GLU*	3.5	4.9	+	-	-	+	
56B GLY*	3.6	2.1	-	-	-	-	
57B GLY*	3.1	29.0	+	-	-	-	
58B GLY*	3.0	29.5	+	-	-	-	
61B PHE	3.8	5.5	-	-	-	+	
62B ARG*	2.6	65.8	+	-	-	+	
63B GLY*	2.7	22.0	+	-	-	-	
64B ALA	4.6	0.7	+	-	-	-	
73B ARG*	5.4	1.6	-	-	-	-	
77B ASP*	2.7	64.9	+	-	-	+	
80B GLY*	3.0	23.6	-	-	-	+	
81B MET*	3.3	23.5	-	-	+	+	
84B THR*	3.9	11.9	-	-	+	-	
137B GLY*	4.0	10.3	+	-	-	-	
138B THR*	2.7	45.5	+	-	-	+	
140B ASN	2.8	22.5	+	-	-	+	
141B PRO*	3.6	0.7	-	-	-	+	
143B PHE*	3.1	26.7	+	-	-	+	
144B THR*	3.4	33.0	-	-	-	+	
145B THR*	2.9	53.1	+	-	+	+	
166B LYS*	5.6	1.2	+	-	-	-	